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Title: 3D Photonic Crystals Build Up By Self-Organization Of Nanospheres

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14. ABSTRACT

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Theoretical Simulation of 3-D Photonic Crystals

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Abstract

Band gap structure is the most important information while studying electromagnetic propagation in photonic crystals. A collection of free software is used to set up an analysis tool system for simulation purpose. Because it is desired for application and has been a technique challenge to fabricate a photonic crystal possessing a complete photonic band gap operates at the optical wavelength regime, we study how to optimize the size and position of band gap from the standpoint of long range order, short range order, and material property. We show in this paper that , decreasing the variance of k points on the first Brillouin zone by choosing an appropriate lattice type and adjusting the lattice parameters is required to the formation of a larger complete photonic band gap, and for easy calculations we defined the variance quantity when the coordinates of high symmetry points are known; a local symmetry distorted along some specific directions always opens and extends the gaps, and the effects of structure inversion are considered from this viewpoint; dielectric contrast should have a optimum value to fulfill the requirements of position and size of gap simultaneously rather than an as-high-as-possible value, to prevent the wavelength shift of gap to a shorter range.

Keyword: photonic crystal, band structure, band gap, simulation, lattice type

1. Introduction

Photonic crystal are periodically dielectric structure which possesses a band gap in which a frequency range of electromagnetic wave is forbidden to propagate, analogous to the electronic band gap in the case of semiconductors. A dielectric that is periodic along three different axes is called a three-dimensional (3D) photonic crystal, and this 3D periodicity would support an omnidirectional photonic band gap (PBG), or so called complete photonic band gap (CPBG). For novel applications, such as lowering thresholds in maintaining population inversions leading to very efficient solid

state devices [1], to fabricate a 3D photonic crystal exhibiting a CPBG in the optical regime has been a technological challenge. Since the wavelength of the band gap scales directly with the lattice constant of the photonic crystal, optical wavelength PBGs require lattice constants less than one micro. Two system of fabrication methods have been set up, one of which is top-down micro- and nano-fabrication, including a variety of lithographic and selective etching techniques [2-4], and holographic methods [5], and models of various lattice structures and building geometry objects have been proposed by using this kind of method, but its process is usually expensive and inefficient, and working frequency on the optical range is difficulty to be achieved. The alternative economically feasible method is bottom-up self-assembly, in which microspheres in colloidal suspension drive themselves into colloidal crystals by either entropic or chemical forces. The resultant crystals have a number of appealing features. They are readily fabricated with large area, controllable thickness up to several hundreds of repeating layers, and submicro lattice parameters. Furthermore, voids within these colloidal crystals can be infiltrated with selective high dielectric constant materials to make inverse structures, fulfilling the combined requirements on the dielectric contrast and the modulation (the total number and the length of periodicity steps) [6]. Colloidal systems of microspheres crystallize either in face-centered cubic (fcc) or in body-centered cubic (bcc) lattices, and for this lack of versatility in lattice type, some new models arranging colloidal crystals into other structures like diamond structure (actually a fcc lattice with two bases) have been proposed [7].

Generally, the size and position of PBG are the two most important parameters while designing a photonic crystal, the former can be measured as gap-to-midgap frequency ratio, and the latter can be measured as central frequency (or wavelength) of gap. In this paper we investigate in detail how PBGs are modified and optimized through consideration in long range order (lattice type and lattice parameters), short range order (local geometry object and its symmetry) and material property (dielectric contrast) by studying simulation results. Some basic and important instructions and principles are derived to be the guiding toward the road of designing and fabricating a photonic crystal with larger CPBG and working frequency on optical regime.

2. Long range order

Considering in long range order includes the strategies of choosing an appropriate lattice type and modifying the lattice parameter to a optimum value. Essentially, distribution variability of the lattice spacings for a lattice with optimized lattice parameters is what counts in the opening and extending of CPBGs. Theoretically we have found that a larger CPBG always need a less variable distribution of lattice spacings for a specific lattice. To estimate this distribution variability one can observes

the geometry or shape of first Brillouin zone (FBZ), and to quantify that one can calculate its variance to get a more precise instruction.

2.1 Lattice spacing and Brillouin zones

In the study of electromagnetic wave propagation in 3D periodically dielectric media, one can combine the source-free Faraday's and Ampere's laws at a fixed frequency ω, recasting the Maxwell's equations in an eigenvalue problem form:

$$\vec{\nabla} \times \frac{1}{\varepsilon} \vec{\nabla} \times \vec{H} = \left(\frac{\omega}{c}\right)^2 \vec{H} \qquad (1)$$

where ε is a periodic dielectric function $\varepsilon(\vec{x}) = \varepsilon(\vec{x} + \vec{R}_i)$ corresponding to a 3D photonic crystal where $\vec{R}_i (i = 1,2,3)$ is the primitive lattice vector , and c is the speed of light in vacuum. Furthermore, by applying the Bloch's Theorem, solutions to Equation (1) can be chosen of the form $\vec{H}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} \vec{H}_{n,\vec{k}}(\vec{x})$ with eigenvalues $\omega_n(\vec{k})$, where $\vec{H}_{n,\vec{k}}$ is a periodic envelope function satisfying:

$$(\vec{\nabla} + i\vec{k}) \times \frac{1}{\varepsilon}(\vec{\nabla} + i\vec{k}) \times \vec{H}_{n,\vec{k}} = \left(\frac{\omega_n(\vec{k})}{c}\right)^2 \vec{H}_{n,\vec{k}} \qquad (2)$$

where $\vec{k}$ is Bloch wavevector. A dispersion relation or band structure diagram is figured out when eigenvalues $\omega_n(\vec{k})$ are plotted versus wavevector $\vec{k}$, and $\omega_n(\vec{k})$ are called nth bands. A CPBG is a range of ω in which there are no propagating solutions of Equation (2) for any $\vec{k}$, and a pseudogap is over a subset of all possible wavevectors, polarizations, and/or symmetries. The method that computes definite-frequency eigenvalues is describe in more detail in [8,9]. Moreover, when calculating eigensolutions, only a set of inequivalent wavevectors closet to the $\vec{k} = 0$ origin, a region called the first Brillouin zone (FBZ), should be considered, because of the periodic function $\omega_n(\vec{k}) = \omega_n(\vec{k} + \vec{G}_j)$ where $\vec{G}_j$ is the primitive reciprocal lattice vector. FBZ can be reduced furthermore into irreducible Brillouin zone (IBZ)

for its symmetry, and corners of IBZ are called high symmetry points. Band extrema almost always occurs at points along paths between adjacent high symmetry points, and band structure diagrams are conventionally plotted at these points.
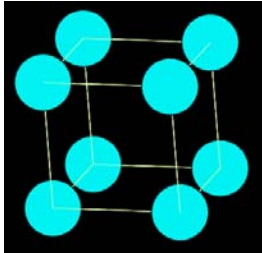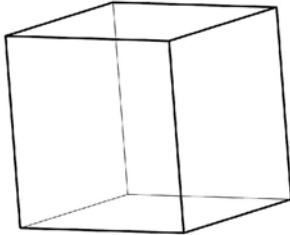
Wavevector $\vec{k}$ can be viewed as lattice point in reciprocal space, or k space, and called k point. A k point with specific direction and magnitude identifies a set of parallel lattice planes with specific orientation and periodicity. A FBZ of a lattice is a set of k points defined as:
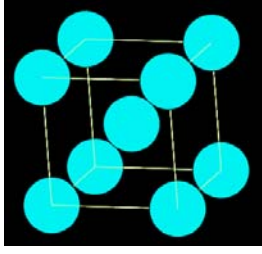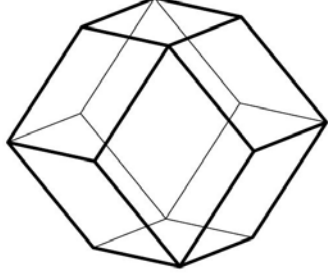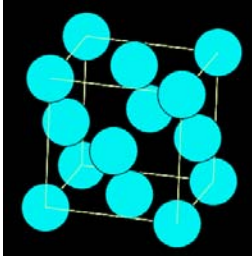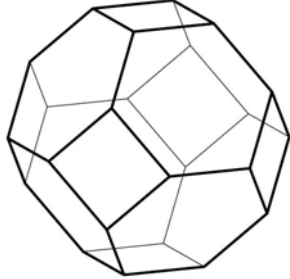
$$K_{lat} = \{\vec{k_i}\}(i = 1,2,3\ldots n) \tag{3}$$

so that K_{lat} can be a collective representation of a crystal by assigning an arbitrary lattice plane to $\vec{k_i}$. It is well known that the gap, or stop band for a k point arise from Bragg's diffraction on a set of planes. For stop bands to overlap over all orientations of these sets of planes, as a result to generate a CPBG, the periodicities (lattice spacings) of these different sets of planes should not be diverse too much, in statistical words, K_{lat} should not have its variability of distribution too large for CPBG formation.

Since K_{lat} is a set of k points on the FBZ for some lattice type, one can estimate the variability of distribution of K_{lat} by the observation of the geometry or shape of a FBZ. The cubic system lattices and their corresponding FBZs are shown in Table 1. It was mentioned by Yablonovitch et al. [10] that a sphere-like FBZ improves the prospects for a forbidden gap to overlap all the way around its surface. It is because the ideal sphere shape of FBZ implies no deviations about the mean of magnitudes of k points, as a result the more sphere-like are the FBZs for some lattices, the more narrow spread distribution of lattice spacings the lattice structures possess. Therefore, we can choose a lattice type as a prototype to fabricate by observing the shape of a FBZ, which indicate how variable the lattice spacings of a lattice distribute.

Table 1. Bravais lattices (cubic system) and their corresponding first Brillouin zones [11,12].

System	Lattice name	Direct lattice	First Brillouin zone
cubic	simple cubic		

body-centered cubic		
face-centered cubic		

2.2 Variance of Lattice spacings

Other than by observing the shapes of FBZs for different lattice types, one can get a more precise control over which lattice is expected to exhibit larger CPBG through calculating the variance of lattice spacings for a specific lattice. Information about variance could be even more useful when fabrication technique only allow the lattice parameters to be adjusted for optimization. We define some quantities as in Table 2. What should be mentioned is for k points on IBZ, one should weight them with corresponding multiplicities to represent all k points on FBZ or lattice planes in all directions, and this calculation procedure is shown evidently in Equation (4) and Equation (5).

Table 2. Quantities defined about lattice spacing, the unit a is lattice constant.

Quantity	Uint	Meaning
K_i	-	an element of the k point set on IBZ
K_{di}	a	lattice spacing or d spacing of K_i
K_{mi}	-	multiplicity of K_i
A_{lat}	a	average of lattice spacings
V_{lat}	a	variance of lattice spacings

A_{lat} and V_{lat} in Table 2 are defined below:

$$A_{lat} = \frac{\sum (K_{di} \times K_{mi})}{\sum K_{mi}} \tag{4}$$

$$V_{lat} = \frac{\sum[(K_{di} - A_{lat})^2 \times K_{mi}]}{\sum K_{mi}} \tag{5}$$

where the subscript *lat* would be replaced by any lattice abbreviation.

A calculation example is given below.

It was proposed by Toader et al. [13] that by means of photolithography and template inversion technique, one can fabricate an inverse type of photonic crystal having the lattice type of simple tetragonal of air slanted pores in high dielectric constant matrix. These types of photonic crystals featured the possession of large CPBGs above 20%, and they were denoted by the symbol SP_n, where n means the numbers of cylinders or so called slanted pores in an unit cell. A more specific symbol $S/[111]$ $[-1-11]^{(0\ 0.5\ 0)}$ represents two cylinders having directions <111> and <-1-11> respectively and apart away with each other at a distance of 0, 0.5, 0 (in unit of lattice constant a) along x, y, z axis respectively.

We take this $S/[111]$ $[-1-11]^{(0\ 0.5\ 0)}$ structure as a calculation example. We set constant the radii of cylinders, but the lattice parameter ratio c/a is permitted to vary. Resultant band structure diagrams are shown serially in Figure 1.
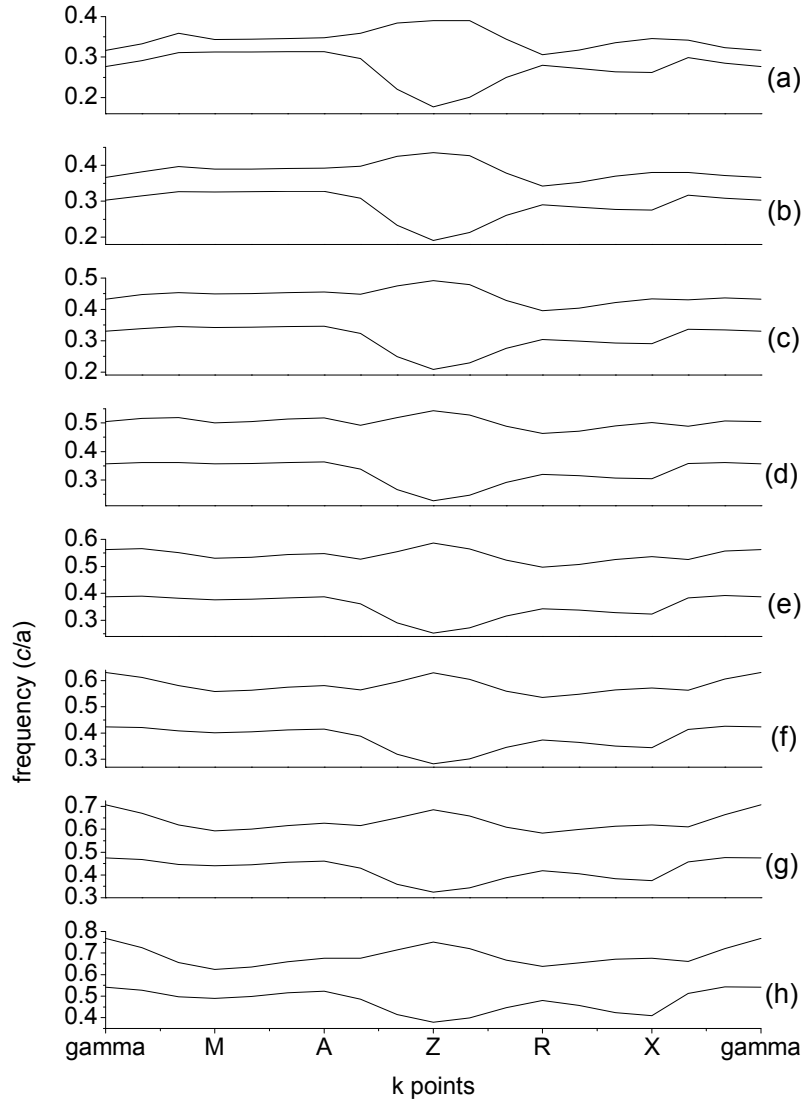
Figure 1. The calculated serial band structures [14] between the lower 4th band and upper 5th band. Calculations are carried out on the simple tetragonal lattice of air slanted pores in high dielectric constant matrix, and the lattice parameter c/a is permitted to vary (c denoted in the frequency c/a is the speed of light in vacuum). The gap sizes are (a) 0 % while c/a = 0.8, (b) 0 % while c/a = 0.9, (c) 13.94% while c/a = 1.0, (d) 20.30% while c/a = 1.1 (e) 22.62% while c/a = 1.2, (f) 23.78% while c/a = 1.3, (g) 24.16% while c/a = 1.4, (h) 13.30% while c/a = 1.5, (i) 4.29 % while c/a =1.6.

It is shown serially in Figure 1 that a CPBG is always closed by inconsistency on frequency range for stop band associated with each k point. On the other hand, flattening of curves (propagating states) above and below the stop band causes the

opening and extending of gap, which actually is a result of decreasing of the variance value. Therefore, variance for simple tetragonal V_{st}, of which general form is defined in Equation (5), could be an important parameter affecting band structure, and it is plotted along with gap size both as a function of lattice parameter ratio c/a in Figure 2. Apparently, the inverse of variance, i.e. $1/V_{st}$, shows a nearly-same variation as gap size when c/a value changes. In conclusion, to achieve a larger size of CPBG, it is the aim to decrease V_{lat} as much as possible.
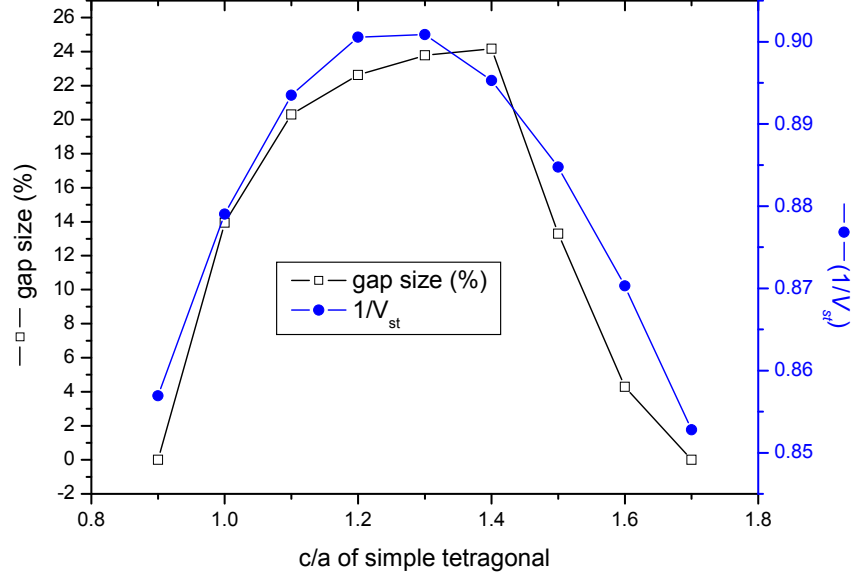
Figure 2. $1/V_{st}(\bullet)$ along with band gap size ($\square$) both as a function of parameter ratio c/a for simple tetragonal of air slanted pores in high dielectric constant matrix.

Another important topic is the position of band gap, because for application purpose, it is desired to design gaps at the frequency range of visible light. Calculation shows that the position (measured in central frequency of gap) is related to the average of lattice spacings, i.e. A_{st}, of which general form is defined in Equation (4), as illustrated in Figure 3.
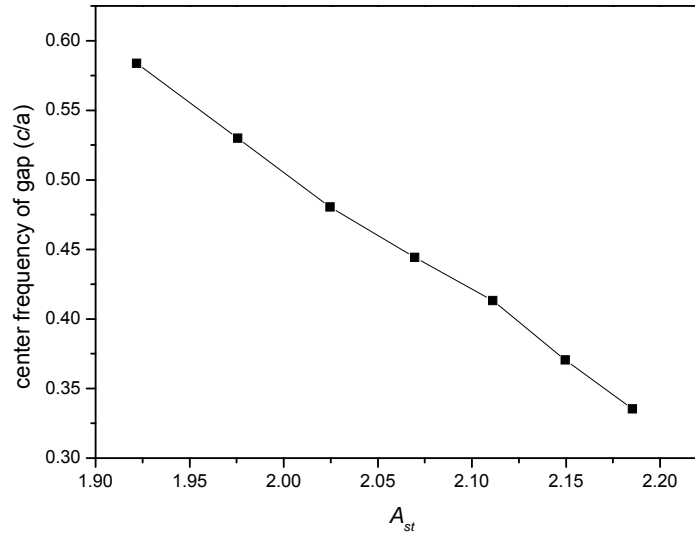
Figure 3. Gap position (measure in central frequency c/a where c is the speed of light in vacuum, and a is lattice constant) as a function of average of lattice spacings for simple tetragonal of air slanted pores in high dielectric constant matrix.

## 3. Short range order

3.1 Local symmetry

Self-assembly colloidal crystal arranged in fcc structure always exhibit gaps only in the <111> direction, and it is shown by vector-wave-band theory [15] that spherical atomic symmetry produced a degeneracy between valence and conduction band at the W point of the Brillouin zone, i.e. <111> direction, allowing only a pseudogap, rather than a CPBG. The degeneracy at the W point could be lifted by distortion of the spherical atoms along the <111> direction [10]. Ho et al. [15] introduced the diamond structure which required tow atoms per unit cell, and Yablonovitch et al. [10] introduced the well-known YGL structure, using a lattice of criss-crossing pores, oriented along the three primitive lattice vectors of the fcc lattice on the sample surface, both structures exhibit CPBGs by distorting the local symmetry of spherical atoms. Afterward, Ho et al. [16] proposed the woodpile structure, assembled by stacking together layers of dielectric rods, giving the symmetry of a face-centered tetragonal lattice, exhibiting a large CPBG. The woodpile and other structures, including layered diamond structure [17], ABC type hexagonal structure [18], and the bicontinuous diamond D level set [19], are in fact all based on the distorted diamond structure. Additionally, other architectures based on the non-diamond structure [20-22] and non-spherical local geometry objects, with relatively less complexity of

microfabrication, were proposed. All these structures suggested that appropriate forms of short range order with breaking symmetries would be essential to the formation of a large CPBG, while maintaining the long range order periodicity.

3.2 Inverse structure

The inverse structures provide another way to the formation of CPBGs by making the relatively high dielectric constant material non-spherical. As shown in Figure 4, the inverted structure for a fcc structure of spheres in a background with dielectric contrast 12 exhibits a CPBG, as illustrated in Figure 4(b), rather than a pseudogap, as illustrated in 4(a), and the gap moves to a higher frequency range than the direct case, a unfavorable shift to the shorter-wavelength operation regime.
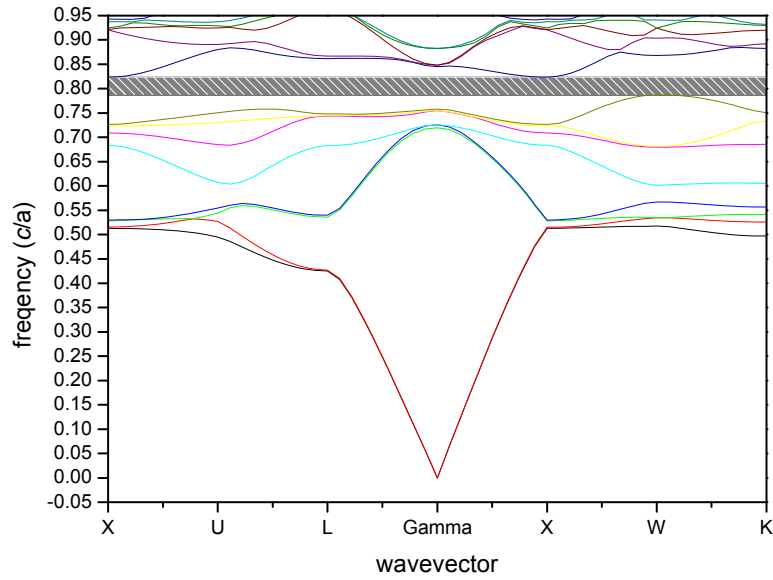
(a)
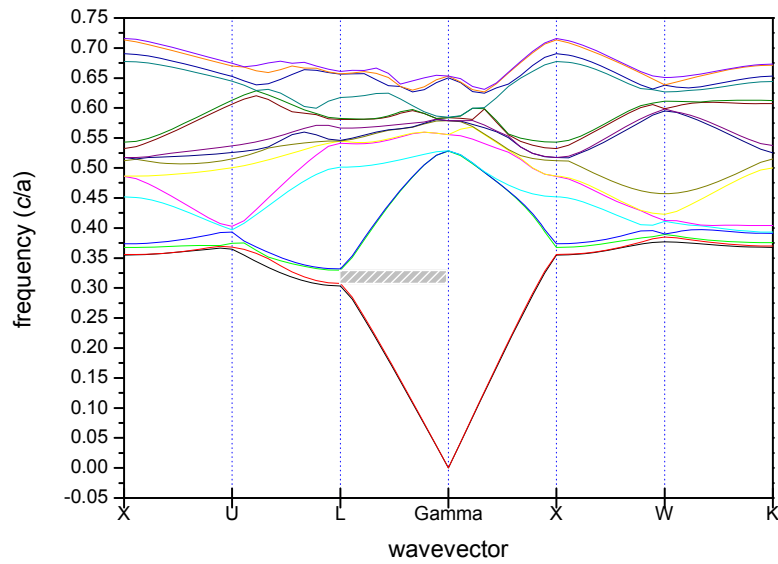
(b)

Figure 4. Calculated band structure for a fcc structure of spheres in a background with dielectric contrast 12. (a) Direct structure exhibiting a pseudogap of 6.90% between the 2nd and 3rd bands, (b) inverse structure exhibiting a CPBG of 4.47% between the 8th and 9th bands.

But for different architecture, the effect of inverse structure is not in the same way. As shown in Figure 5, the inverted diamond structure has a smaller gap size than the direct one, it is maybe caused by the contrary effect to the sphere-distorted diamond structure that has taken the broadening effect to the PBG.
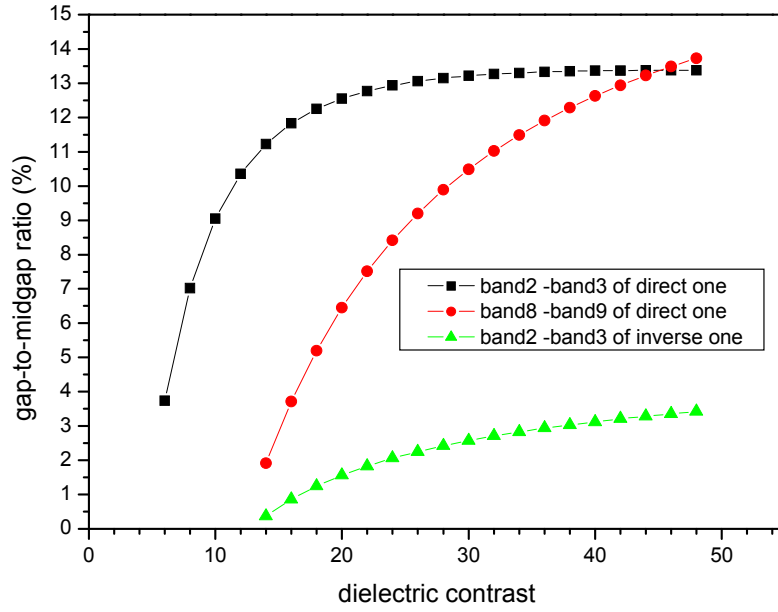
Figure 5. Gap size (gap-to-midgap ratio) as a function of dielectric contrast for direct structure and inverse structure. The architecture is a close-packed diamond structure. (-▦-) The gap between the 2nd and 3rd bands for direct structure, (-●-) the gap between the 8th and 9th bands for direct structure, (-▲-) the gap between the 2nd and 3rd bands for inverse structure.

However, inverse diamond structures of overlapping spheres rapidly change the gap size to a larger one, as illustrated in Figure 6 and Figure 7, and it is shown from Figure 7(b) that a CPBG operated at optical wavelength could be achieved if the inverted diamond structure with optimum r/a ratio (r is the radius of sphere) could be fabricated with more feasible techniques.

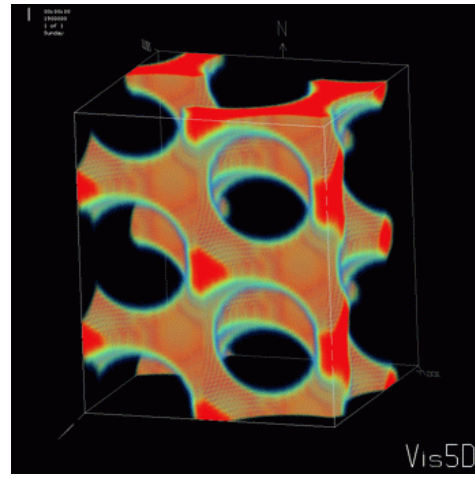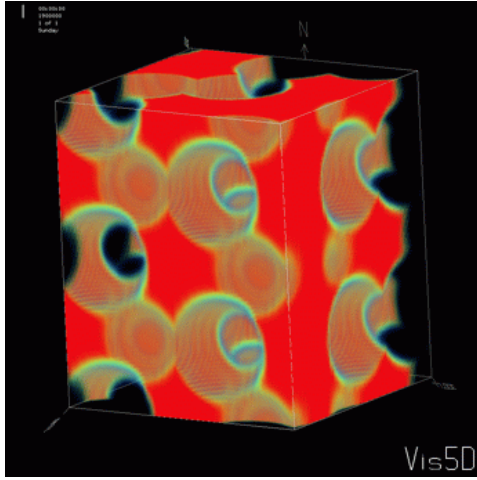(a)   (b)
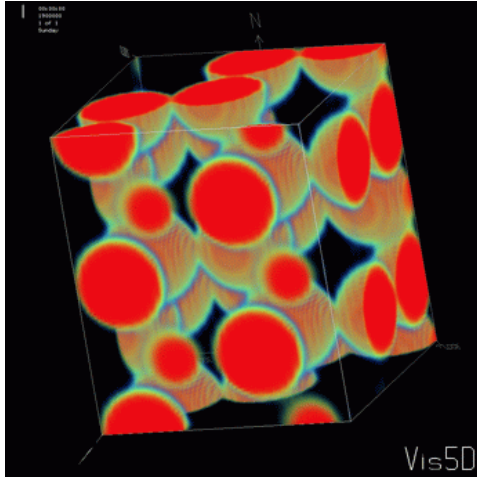
(c)
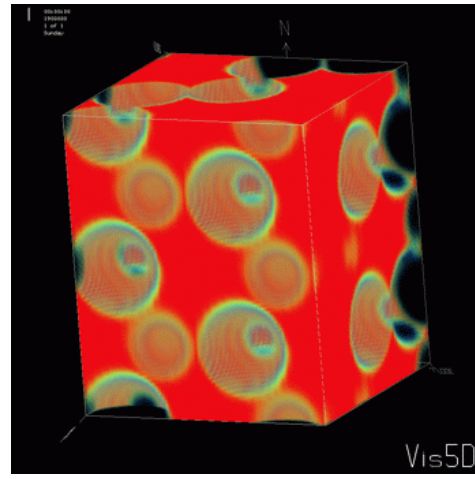
(d)

Figure 6. Direct and inverse diamond structures with various r/a, where r is radius of sphere and a is lattice constant. When (a) the direct diamond structure is close-packed, gap size is 10.36% of the central frequency, (b) the inverse diamond structure is close-packed, without a CPBG, (c) the inverse structure is composed of overlapping spheres with r/a = 0.240, gap size is 7.90%, (d) the inverse structure is composed of overlapping spheres with r/a = 0.325, gap size is 26.92%.
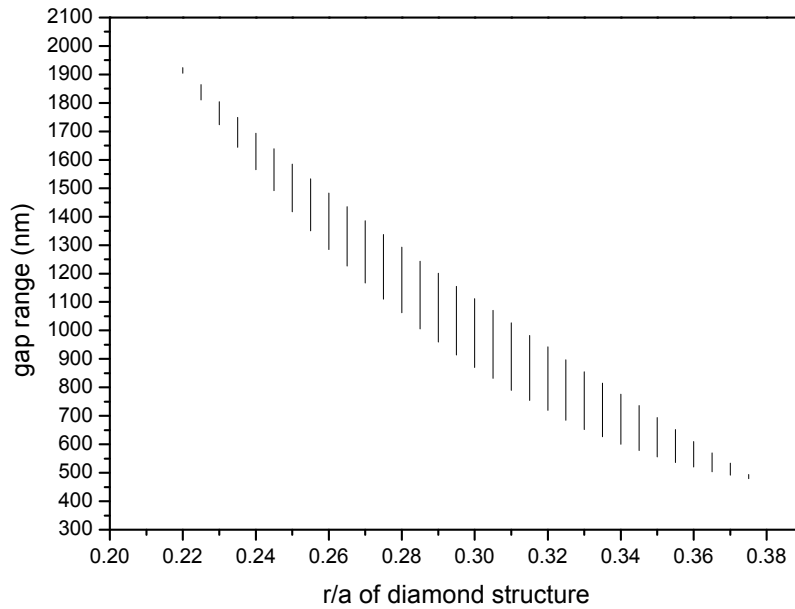
(a)
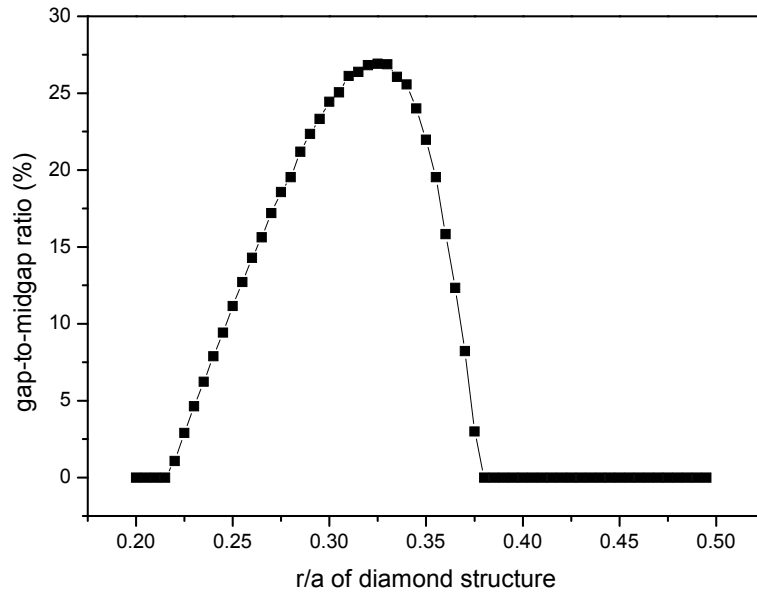
(b)

Figure 7. (a) Gap size and (b) gap range as a function of the r/a ratio of the inverted diamond structure where r is the radius of spheres and a is lattice constant (set to 150nm). The dielectric contrast is set to 12.

4. Material property: dielectric constant

Opal colloidal crystal only permits a pseudogap rather than a CPBG always because of its low dielectric contrast. However, since the interstitial spaces within opals are empty, they can be infiltrated with relatively high dielectric constant materials, and after removal of the opal template, one get inverted opals possessing higher dielectric contrast than opals. A variety of inorganic materials, including metal oxide [22-27], metals [28-30], semiconductors [31-34], were prepared to make inverted structures. It is pointed out that the width of gap will increase with dielectric contrast [35,36]. But the increase rate is in a decreasing manner for a CPBG, take the opal-like close-packed diamond structure exhibiting CPBGs as an example, as illustrated in Figure 8, the size of gap between 2nd and 3rd bands almost stop to increase when dielectric contrast is larger than 20. Although it is interesting that the higher gap, i.e. the gap between 8th and 9th bands broaden its width in a continually increasing manner, even with a larger gap size than the lower one when dielectric contrast exceed about 45.
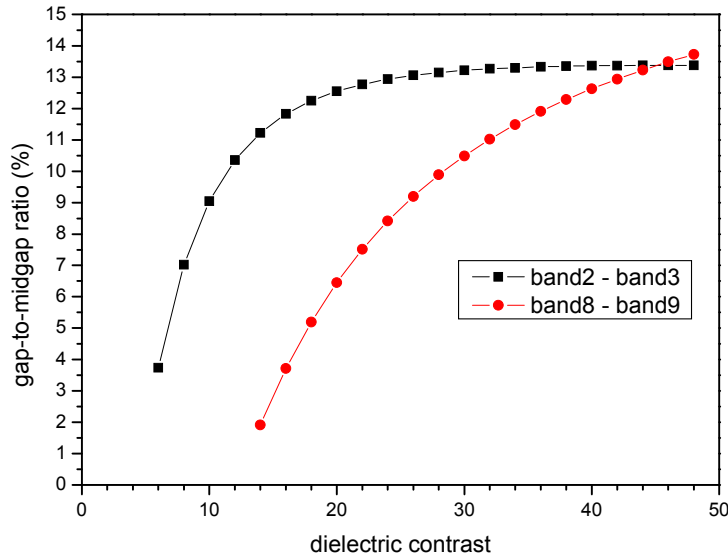

Figure 8. Gap size (gap-to-midgap ratio) as a function of dielectric contrast for an opal-like close-packed diamond structure of dielectric spheres in air background exhibiting CPBGs between (-▓-) 2nd and 3rd bands and (-●-) 8th and 9th bands.

However, it is a different case for a pseudogap typically exhibited by an opal-like close-packed simple fcc structure. As illustrated in Figure 9, the maximum gap size appears when dielectric contrast is about 6, and the higher order gap except that

between the 5th and 6th bands would be ignored because their extremely small size for the common range of dielectric contrast.
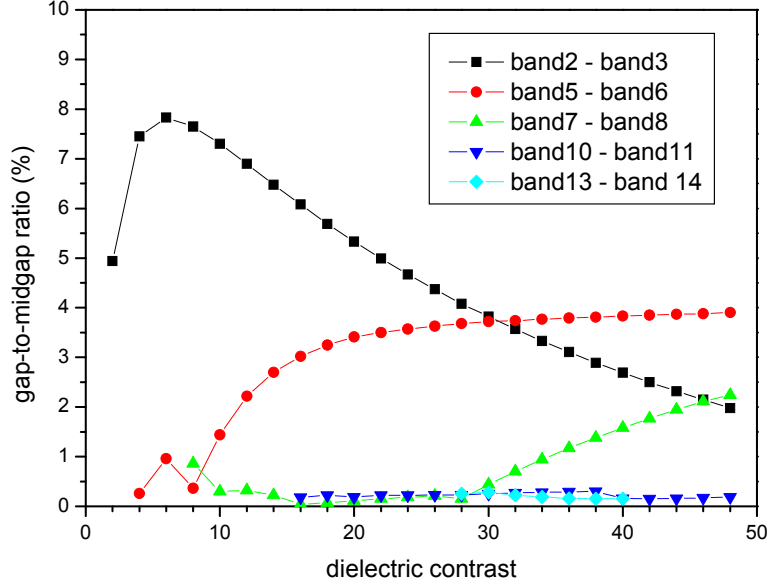

Figure 9. Gap size (gap-to-midgap ratio) as a function of dielectric contrast for an opal-like close-packed fcc structure of dielectric spheres in air background exhibiting pseudogaps in the <111> direction between the (-▦-) 2nd and 3rd bands, (-●-) 5th and 6th bands, (-▲-) 7th and 8th bands ,(-▼-) 11th and 12th bands, and (- -) 13th and 14th bands.

Changing the dielectric contrast not only affect the size of PGB, but also the position. Increasing the dielectric contrast would shift the operation wavelength to a shorter range, both for the pseudogap and CPBG case, as illustrated in Figure 10 and Figure 11 respectively, which is not a favorable tendency while optical regime is desired. As a result, an appropriate value of dielectric contrast both fulfill the requirements of large enough gap and longer enough operation wavelength is needed, and simulations could easily do this kind of optimization work.
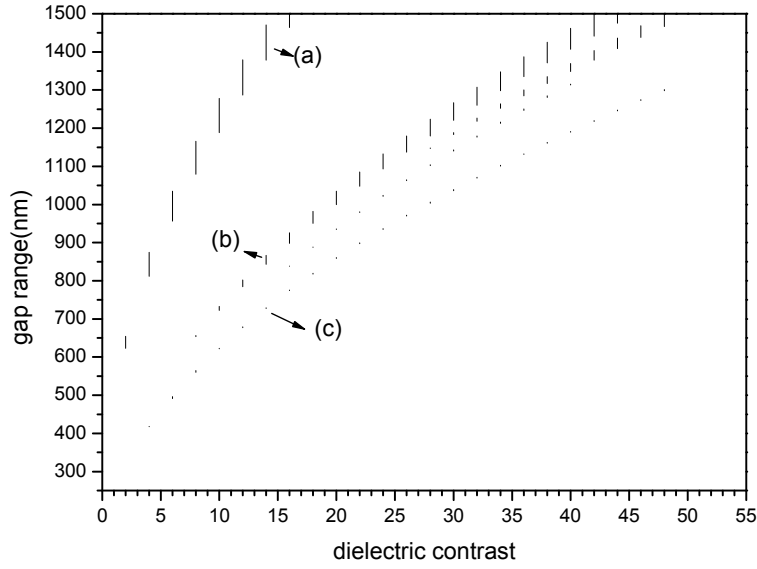
Figure 10. Gap range as a function of dielectric contrast for an opal-like close-packed fcc structure of dielectric spheres in air background exhibiting pseudogaps between the (a) 2nd and 3rd bands with gap-to-midgap ratio of 6.48% and range from 1378nm to 1471nm, (b) 5th and 6th bands with gap-to-midgap ratio of 2.70% and range from 843nm to 866nm, and (c) 13th and 14th bands with gap-to-midgap ratio of 0.22% and range from 727nm to 729nm, when sphere radius is set to 150nm and its dielectric contrast is set to 14.
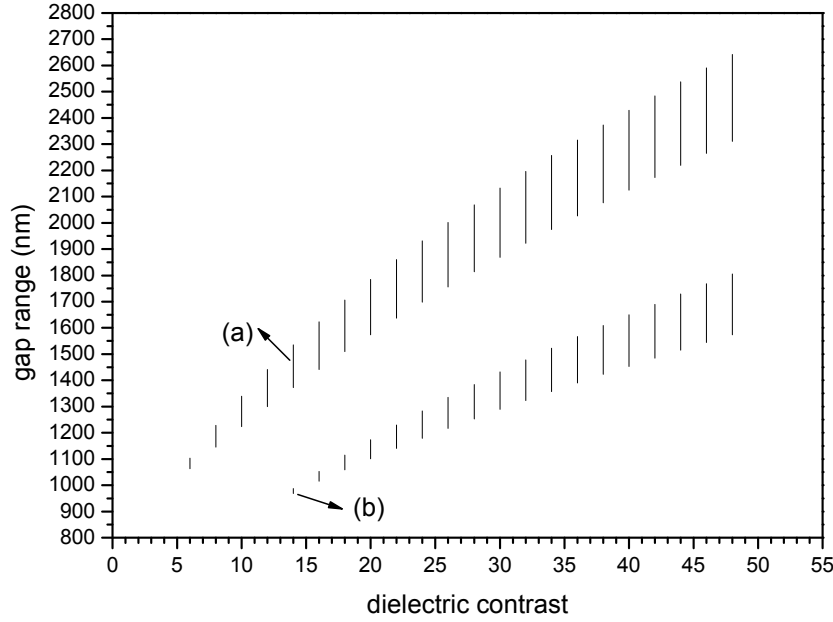
Figure 11. Gap range as a function of dielectric contrast for an opal-like close-packed diamond structure of dielectric spheres in air background exhibiting CPBGs between the (a) 2nd and 3rd bands with gap-to-midgap ratio of 11.23% and range from 1371nm to 1535nm, (b) 8th and 9th bands with gap-to-midgap ratio of 1.91% and range from 968nm to 987nm, when sphere radius is set to 150nm and its dielectric contrast is set to 14.

5. Set-up of analysis tools

The main simulation program calculating the dispersion relation, i.e. band structure, of photonic crystal is MIT Photonic-Bands (MPB) [14], developed by Steven G. Johnson. It computes the definite-frequency eigenstates of Maxwell Equations in periodic dielectric structures for arbitrary wavevectors, using fully-vectorial and three-dimensional methods. The computer operation system at which MPB runs would be FreeBSD [37] because its easy installation process. Other assistant tools include Perl [38], for output processing and parameter controlling of main program, and Vis5D [39], for visualization of dielectric functions. All these programs were released under the GNU general public license [40]. Additionally, the coordinates of high symmetry points on the irreducible Brillouin zone for various lattice are calculated and indexed by XCrysDen [11], of which output is supplied as input of MPB main program. These tools' name along with their versions , licenses, and functions are listed in Table 5.

Table5. Simulation tools' name along with their versions , licenses, and functions.

tools	versions	licenses	functions
FreeBSD	5.4 Release	GNU General Public License GNU Library Public License	computer operation system
MPB	1.4.2_1	GNU General Public License	band structure computation
Perl	5.8.7 Release	Artistic License / GNU General Public License	output processing and parameter controlling
Vis5D+	1.2.1_3	GNU General Public License	visualization of dielectric function
XCrySDen	1.4.1	GNU General Public License	graphing of Brillouin Zone and indexing of high symmetry points

6. Conclusion

We use the MPB main program along with other assistant tools to compute the dispersion relation, i.e. band structure, and study how to optimize the size and position of photonic band gap. While a complete photonic band gap operates on the optical wavelength regime is required for application purpose, we give some basic principles of designing from the viewpoints of long range order, short range order, and material property. We show in this paper that , decreasing the variance of k points on the first Brillouin zone by choosing an appropriate lattice type and adjusting the lattice parameters is required to the formation of a larger complete photonic band gap, and for easy calculations we defined the variance quantity when the coordinates of high symmetry points are known; a local symmetry distorted along some specific directions always opens and extends the gaps, and the effects of structure inversion are considered from this viewpoint; dielectric contrast should have a optimum value to fulfill the requirements of position and size of gap simultaneously rather than an as-high-as-possible value, to prevent the wavelength shift of gap to a shorter range.

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